

## Limitations on a combined phonon–non-phonon mechanism for superconductivity in $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$

T.W. Barbee III

*L-412, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550, USA*

Marvin L. Cohen

*Department of Physics, University of California, Berkeley, CA 94720, USA  
and Materials Sciences Division, Lawrence Berkeley Laboratory, Berkeley, CA 94720, USA*

and

David R. Penn

*Radiation Physics Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA*

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Despite the large number of theories proposed to explain high-temperature superconductivity, no clear explanation of its origin exists. Experimental data such as the isotope effect  $\alpha$  and the gap ratio  $2\Delta/k_B T_c$  can be used to constrain possible models for high-temperature superconductivity. We consider a class of models which contain contributions to pairing from phonons and also from another unspecified boson, and place limitations on such models in light of these experimental data and recent results derived from photoemission data for  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$ .

Approximately four years after the discovery [1,2] of high-temperature superconductivity (HTS) in oxides, the nature of the mechanism(s) responsible for HTS remains unclear. Many theories have been designed to explain the unusual properties of these materials. These theories range from adaptations of the conventional phonon-mediated theories [3,4] to more exotic theories in which phonons play no role. For some high- $T_c$  superconductors, such as Ba–K–Bi–O, there is some experimental evidence that the standard phonon-mediated model of superconductivity may be valid. For the higher- $T_c$  cuprates, the situation is less clear.

Measurements of superconducting properties of the oxides such as the isotopic effect  $\alpha$  and the superconducting energy gap ratio  $2\Delta/k_B T_c$  can help distinguish among the many theories which predict high-transition temperatures in the superconducting oxides. One possible HTS theory is the combined

phonon–non-phonon mechanism, in which both phonons and another as yet unknown boson contribute to the pairing of the electrons. By using experimental data, we have placed constraints [5] on the range of parameters in such a model for several of the oxides.

Recently, Mueller et al. analyzed [6] temperature-dependent photoemission data [7] for  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$  and found evidence for such a combined mechanism with extremely strong coupling ( $\lambda \approx 9$ ) to a boson of low characteristic energy (10 meV). In this paper, we consider such a mechanism in light of the other experimental data, such as the isotope effect  $\alpha$  and the gap ratio  $2\Delta/k_B T_c$ . The available experimental data indicate that the transition temperature  $T_c = 91$  K and the oxygen isotope effect [8]  $0.048 > \alpha_O > 0.034$ . Depending on the experimental technique, the gap ratio  $2\Delta/k_B T_c$  is found to vary widely with results ranging from 3.3 up to 8. The ex-

periment in which the value  $2\Delta/k_B T_c = 3.3$  was found also showed an unusual (non-BCS [3]) temperature dependence of  $\Delta(T)$ .

In our calculations, we have used an electron-phonon interaction spectrum  $\alpha^2 F(\omega)$  derived from neutron scattering data [9] under the assumption that the electron-phonon coupling  $\alpha^2$  is independent of energy. As a test of this spectrum, we have also used an  $\alpha^2 F(\omega)$  derived from a theoretical calculation [10] of the phonon density of states  $F(\omega)$  under the assumption of a constant  $\alpha^2$ . We find only small differences in the results using the two different spectra.

The major phonon peaks in the neutron scattering measurement and in the theoretical calculation are modeled by narrow Lorentzians of the form

$$\alpha^2 F(\omega) = \alpha^2 \sum_i \frac{A_i \Gamma_i^2}{(\omega - \omega_i)^2 + \Gamma_i^2}, \quad (1)$$

where  $A_i$  is the amplitude of peak  $i$ ,  $2\Gamma_i$  its width, and  $\omega_i$  its central frequency. The parameters of the Lorentzians used are given in table 1. All of these peaks are assumed to be associated with the oxygens. The phonon coupling strength  $\lambda_{ph}$  may be adjusted by varying the assumed value of  $\alpha^2$ . A non-phonon peak of strength  $\lambda_{el}$  and energy  $\omega_{el}$  is then added to the spectrum to yield the  $\alpha^2 F(\omega)$  used in the calculations. The Coulomb pseudopotential  $\mu^*$  is chosen to be  $\mu^*(\langle \omega_{ph} \rangle) = 0.13$ , where  $\langle \omega_{ph} \rangle$  is the average phonon frequency. The results are not sensitive to the choice of  $\mu^*$ . In the calculation of the isotope effect, the peaks identified as oxygen related in the neutron scattering study are assumed to contribute to the oxygen isotope effect, since the other peak is assumed to be independent of the oxygen mass. De-

tails of the isotope effect calculations are published elsewhere [5]. As was done in ref. [5], the observed  $T_c$  and isotope effect  $\alpha_O$  are used as constraints on the three parameters  $\lambda_{ph}$ ,  $\lambda_{el}$ , and  $\omega_{el}$ . We choose  $\omega_{el}$  as the free parameter, and obtain the coupling strengths  $\lambda_{el}$  and  $\lambda_{ph}$  as functions of  $\omega_{el}$ . The total coupling  $\lambda$  is given by  $\lambda = \lambda_{ph} + \lambda_{el}$ .

Fig. 1 shows the results of our calculations for  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$  for  $T_c = 7.5$  meV (87 K) and  $\alpha_O = 0.05$  using the spectrum derived from the neutron scattering data [9]. We find that  $\lambda_{ph} < 0.45$  over the entire range of  $\omega_{el}$ . Therefore, if  $\lambda_{ph}$  is more than 0.45, a combined phonon-non-phonon mechanism within Eliashberg theory would be excluded for  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$ . Experimentally [11],  $\lambda_{ph} = 0.8 \pm 0.4$  which greatly exceeds this limit. It follows that a combined mechanism with high-energy bosons can be excluded as  $\lambda_{ph} < 0.1$  for  $\omega_{el} > 100$  meV. However, a combined mechanism with low-energy bosons cannot be excluded due to the large error bars on the experimental value of  $\lambda_{ph}$ .

Fig. 2 shows the gap ratio  $2\Delta/k_B T_c$  and total coupling strength  $\lambda$  for  $\omega_{el}$  below 50 meV. At the smallest values of  $\omega_{el}$ ,  $\lambda$  increases dramatically with decreasing  $\omega_{el}$ . For instance, changing  $\omega_{el}$  from 20 to 10 meV increases  $\lambda$  from 6.5 to 21.5 and  $2\Delta/k_B T_c$  increases from about 7 to 8.8. Therefore, a combined mechanism with extremely strong coupling to a low-energy boson is consistent with the data for  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$ .

In their fit of  $\alpha^2 F(\omega)$  to the photoemission data, Mueller et al. found a strong peak in  $\alpha^2 F(\omega)$  at 10 meV and a total coupling strength of  $\lambda \approx 9$  and a gap ratio  $2\Delta/k_B T_c \approx 5$ . We find that the predicted  $\lambda$  is much greater than values observed in the conven-

Table 1

The parameters of the two electron-phonon interaction spectra used in the calculations are shown. The spectra are obtained by summing Lorentzians of amplitude  $A_i$  and half-width  $\Gamma_i$  centered at  $\omega_i$ . In the calculation of the isotope effect, all of these peaks are assumed to be related to the movement of oxygen atoms.

Theoretical (ref. [10])			Neutron scattering (ref. [9])		
$\omega_i$ (meV)	$A_i$	$\Gamma_i$ (meV)	$\omega_i$ (meV)	$A_i$	$\Gamma_i$ (meV)
57	3.0	2.0	31	4.0	2.0
67	4.0	1.0	43	3.0	2.0
77	2.3	1.0	58	2.0	1.0
			72	2.0	2.0

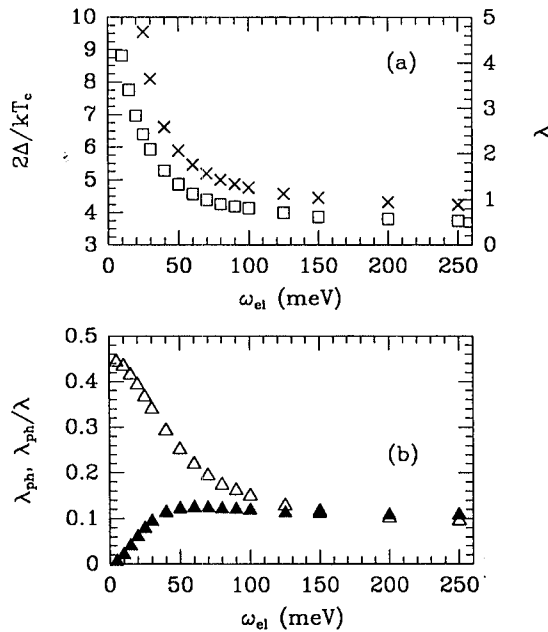


Fig. 1. Calculated parameters plotted against the characteristic energy  $\omega_{el}$  of the non-phonon interaction giving measured values of  $\alpha_O$  and  $T_c$  appropriate for  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$ . (a) Total coupling  $\lambda = \lambda_{ph} + \lambda_{el}$  (crosses, right-hand scale), and the gap ratio  $2\Delta/k_B T_c$  (squares, left-hand scale). (b) Phonon-mediated coupling  $\lambda_{ph}$  (open triangles) and the fraction of phonon-mediated coupling  $\lambda_{ph}/\lambda$  (filled triangles). Hence  $\lambda_{ph} < 0.45$  for  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$ .

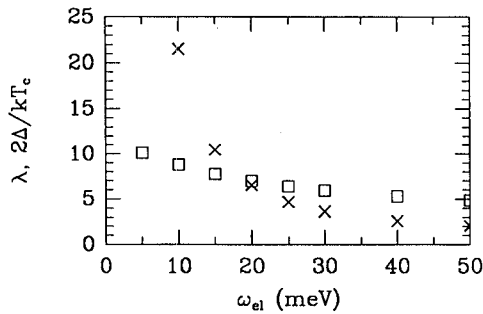


Fig. 2. Expanded view of fig. 1a for boson energies between 0 and 50 meV. The symbols used are the same as in fig. 1a.

tional superconductors and  $2\Delta/k_B T_c$  is large, but the precise values of  $\lambda$  and  $2\Delta/k_B T_c$  disagree with those of Mueller. The disagreement may arise from differences in the phonon-based component of  $\alpha^2 F(\omega)$  or in our use of the isotope effect as a constraint.

In  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$ ,  $\alpha_O$  is between [8] 0.034 and

0.048. Calculations with  $\alpha_O = 0.025$  rather than 0.05 as used above yield basically the same results, except that  $\lambda_{ph}(\omega_{el})$  is decreased to about half its previous value over the entire range of  $\omega_{el}$ , while the calculated values of  $\lambda_{el}$  increase by a few percent. Thus,  $\lambda$  only varies by a few percent when  $\alpha_O$  is varied between 0.025 and 0.05, and the constraint on  $\lambda_{ph}$  is more severe for smaller  $\alpha_O$ .

Since the experimental values of  $2\Delta/k_B T_c$  vary widely (from  $3.3 \pm 0.3$  in a reflectivity measurement [12] to  $8 \pm 1.4$  from photoemission [13]), it is difficult to use the calculated values of  $2\Delta/k_B T_c$  to constrain the range of  $\omega_{el}$ . We note that the large gap ratio observed by photoemission is consistent with a combined phonon-non-phonon mechanism with  $10 < \omega_{el} < 20$  meV.

We note that the results presented in this work and in ref. [6] are based on the assumptions that  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$  is a three-dimensional homogeneous isotropic superconductor with harmonic phonons, that Migdal-Eliashberg theory holds for pairing due to bosons other than phonons, and that the ground state of the electrons is a Fermi liquid.

In this calculation, we have found that a combined phonon-non-phonon mechanism with strong coupling to a low-frequency boson is consistent with the values of  $\alpha_O$  and  $2\Delta/k_B T_c$  found in  $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_x$ . Such a mechanism would also account for the linearity of the electrical resistivity at low temperatures [14].

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